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Collective excitations of Bose-Einstein-condensed gases at finite temperatures

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We have applied the Popov version of the Hartree-Fock-Bogoliubov (HFB) approximation to calculate the finite-temperature excitation spectrum of a Bose-Einstein condensate (BEC) of ^{87}Rb atoms. For lower values of the temperature, we find excellent agreement with recently published experimental data for the JILA time-averaged orbiting potential trap. In contrast to recent comparison of the results of HFB-Popov theory with experimental condensate fractions and specific heats, there is disagreement of the theoretical and recent experimental results near the BEC phase transition temperature. [S1050-2947(98)50701-9]

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Laboratory realizations of gaseous Bose-Einstein condensates (BECs) [1–3] have prompted vigorous experimental [4] investigations of the temperature-dependent properties of these mesoscopic quantum systems. The current theoretical interest in such condensates derives, in part, from the fact that experimental tests of many-body theories that are thought to apply to BEC — a phenomenon occurring in many areas of physics — can now be performed. An accurate theory of such systems is therefore of fundamental interest, and will also have practical applications. In this Rapid Communication, we explore the limits of validity of the simplest temperature-dependent mean-field theory — a simplified version of the Hartree-Fock-Bogoliubov (HFB) approximation originally introduced by Popov [5] — by presenting a comparison with experiment of this theory's predictions for condensate excitation spectra at $T>0$.

Condensate properties predicted by such theories include condensate and thermal-atom spatial density profiles, condensate fractions, specific heats, and excitation frequencies. Of these properties, excitation spectra provide the most sensitive test of the applicability of competing theories, since the other quantities listed depend on sums over states and are thus insensitive to small errors in the excitation spectrum. One example of this can be found in the approach of zero-temperature excitation frequencies to the Thomas-Fermi limit (i.e., the limit $N_0\rightarrow\infty$, where N_0 is the number of condensate atoms) as N_0 increases. For ^{87}Rb condensates confined in the JILA time-averaged orbiting potential (JILA TOP) trap where $N_0>4000$ atoms, the Thomas-Fermi predictions for spatial density profiles are extremely accurate while low-order excitation frequencies can differ by as much as 10%.

There is good *a priori* reason to expect that the HFB-Popov theory should provide good predictions of experimental T-dependent collective excitation frequencies. Measurements of zero-temperature frequencies [6] exhibited excellent agreement with the predictions of zero-temperature, mean-field theory [7]. Furthermore, semiclassical variants of the HFB-Popov theory have exhibited excellent agreement with experiment for T-dependent condensate fractions and specific heats for temperatures up to near T_c [9]. The HFB-Popov theory is a finite-temperature extension of mean-field theory that provides self-consistent treatment of the condensed and thermal components of the gas and that should describe the linear response of the condensate to small-amplitude mechanical disturbances [10].

Although the HFB-Popov equations have been derived elsewhere [10,11], we shall briefly state the physics behind the basic equations here. The confined Bose gas is portrayed as a thermodynamic equilibrium system under the grand-canonical ensemble whose thermodynamic variables are N, the total number of trapped atoms, T, the absolute temperature, and either N_0 or μ, the chemical potential. The system Hamiltonian has the form

$$K\equiv H-\mu N=\int d\mathbf{r}\;\hat{\psi}^{\dagger}(\mathbf{r})(H_0-\mu)\hat{\psi}(\mathbf{r})+\frac{U_0}{2}\int d\mathbf{r}\;\hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}),\qquad(1)$$

where $\hat{\psi}(\mathbf{r})$ is the Bose field operator that annhililates an atom at position $\mathbf{r}$ and $H_0=(-\hbar^2/2M)\nabla^2+V_{\rm trap}(\mathbf{r})$ is the

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bare trap Hamiltonian. For the system treated here, the trap potential $V_{\rm trap}(\mathbf{r})=M(\omega_\rho^2\rho^2+\omega_z^2z^2)/2$, where M is the atomic mass, and ω_ρ and ω_z are the radial and axial trap frequencies, respectively. The quantity $U_0=4\pi\hbar^2a/M$ is a measure of the interaction strength between atoms, with a being the scattering length for zero-energy binary atomic collisions, taken to be $109a_0$ for ^{87}Rb [12], where a_0 is the Bohr radius.

The Bose field operator is decomposed into a c-number condensate wave function plus an operator describing the noncondensate part, $\hat{\psi}(\mathbf{r})=N_0^{1/2}\phi(\mathbf{r})+\tilde{\psi}(\mathbf{r})$, and inserted into Eq. (1). When terms cubic and quartic in $\tilde{\psi}(\mathbf{r})$ are treated within the mean–field approximation the grand-canonical Hamiltonian reduces to a sum of four terms: $K=K_0+K_1+K_1^\dagger+K_2$. The first term K_0 is a c number, the second and third terms are linear in $\tilde{\psi}(\mathbf{r})$ and $\tilde{\psi}^\dagger(\mathbf{r})$ and the last term is quadratic in these quantities. It is easy to show that the linear terms vanish identically if $\phi(\mathbf{r})$ satisfies the generalized Gross-Pitaevskii (GP) equation

$$\{H_0+U_0[N_0|\phi(\mathbf{r})|^2+2\tilde{n}(\mathbf{r})]\}\phi(\mathbf{r})=\mu\phi(\mathbf{r}), \qquad (2)$$

where $\tilde{n}(\mathbf{r})$ is the density of noncondensate atoms. Note that the condensate wave function is normalized to unity.

The term K_2 has the form

$$K_2=\int d\mathbf{r}\ \tilde{\psi}^\dagger(\mathbf{r})\mathcal{L}\tilde{\psi}(\mathbf{r})+\frac{N_0U_0}{2}\int d\mathbf{r}[\phi(\mathbf{r})]^2\tilde{\psi}^\dagger(\mathbf{r})\tilde{\psi}^\dagger(\mathbf{r}) + \frac{N_0U_0}{2}\int d\mathbf{r}[\phi^*(\mathbf{r})]^2\tilde{\psi}(\mathbf{r})\tilde{\psi}(\mathbf{r}). \qquad (3)$$

where $\mathcal{L}\equiv H_0+2U_0n(\mathbf{r})-\mu$ and $n(\mathbf{r})=N_0|\phi(\mathbf{r})|^2+\tilde{n}(\mathbf{r})$ is the total trapped-atom density. The term K_2 can be diagonalized by the Bogoliubov transformation,

$$\tilde{\psi}(\mathbf{r})=\sum_j\ [u_j(\mathbf{r})\alpha_j+v_j^*(\mathbf{r})\alpha_j^\dagger], \qquad (4)$$

if the quasiparticle amplitudes $u_j(\mathbf{r})$ and $v_j(\mathbf{r})$ satisfy the coupled HFB-Popov equations:

$$\begin{aligned}\mathcal{L}u_j(\mathbf{r})+N_0U_0|\phi(\mathbf{r})|^2v_j(\mathbf{r})&=E_ju_j(\mathbf{r}),\\ \mathcal{L}v_j(\mathbf{r})+N_0U_0|\phi(\mathbf{r})|^2u_j(\mathbf{r})&=-E_jv_j(\mathbf{r}).\end{aligned} \qquad (5)$$

The α_j and $\alpha_j^\dagger$ are quasiparticle annihilation and creation operators that satisfy the usual Bose commutation relations.

The density of the thermal component of the gas is $\tilde{n}(\mathbf{r})\equiv\langle\tilde{\psi}^\dagger\tilde{\psi}\rangle$, and thus can be written in terms of the quasiparticle amplitudes as

$$\tilde{n}(\mathbf{r})=\sum_j\ \{[|u_j(\mathbf{r})|^2+|v_j(\mathbf{r})|^2]N_j+|v_j(\mathbf{r})|^2\}, \qquad (6)$$

where $N_j=(e^{\beta E_j}-1)^{-1}$ is the Bose-Einstein factor, and $\beta=(k_{\rm B}T)^{-1}$ with $k_{\rm B}$ the Boltzmann constant. The total number of trapped atoms, N, is given by

$$N=\int d\mathbf{r}n(\mathbf{r})=N_0+\int d\mathbf{r}\tilde{n}(\mathbf{r}). \qquad (7)$$

Our version of Eq. (5) differs from that of Ref. [13] via a sign change in the definition of $v_j(\mathbf{r})$.

Equations (2), (5), (6), and (7) form a closed system of equations that we have referred to as the "HFB-Popov" equations. We have numerically solved these equations under conditions appropriate to ^{87}Rb atoms confined in the JILA TOP trap [14]. We choose our state variables to be $\{T,\mu,N\}$, fix T and μ, and then determine N by solving the HFB-Popov equations. This is equivalent to the alternative triple of state variables $\{T,N_0,N\}$, since there is a one-to-one relationship between N_0 and μ.

We have solved the HFB-Popov equations by an iterative procedure, each cycle of the iteration consisting of two steps. In the first step of each cycle, we solve Eq. (2) for new values of $\phi(\mathbf{r})$ and N_0 with a basis-set approach as described previously [15] using $\tilde{n}(\mathbf{r})$ obtained in the previous cycle. In the second step, we solve Eqs. (5) using $\tilde{n}(\mathbf{r})$ from the previous cycle, and the newly generated values of $\phi(\mathbf{r})$ and N_0. With the quasiparticle amplitudes expanded in the trap basis, Eqs. (5) yield a generalized matrix eigenvalue problem for the basis-set coefficients. We recast the generalized matrix eigenvalue problem by using a decoupling transformation consisting of taking the sum and difference of Eqs. (5). This transformation is equivalent to that of Hutchinson *et al.* [13], except that it is expressed in terms of basis set expansion coefficients. Completion of this step yields the $\{u_j(\mathbf{r}),v_j(\mathbf{r})\}$, and E_j which are used in Eq. (6) to update $\tilde{n}(\mathbf{r})$. Equation (7) then updates the total number of trapped atoms N. Convergence is reached when the change in N from one cycle to the next is smaller than a specified tolerance. To obtain converged results at high temperatures, we add a correction to the total number of atoms N at each iteration cycle. High-energy quasiparticle eigenfunctions have negligible overlap with the condensate wave function, so their presence in the thermal sum of Eq. (6) does not significantly modify the low-lying excitation frequencies, but does contribute to the value of N.

We have checked the accuracy of our numerical work by writing two independent codes, which produce identical answers. The ideal-gas result is recovered when we set $a=0$, and we have reproduced the results reported in Ref. [13]. We now discuss the comparison of this approach with experiment.

Figure 1 compares the experimental [14] excitation spectrum of ^{87}Rb in the JILA TOP trap vs our HFB-Popov results for the $m=0$ and $m=2$ modes. The abscissa is the scaled temperature $T'=T/T_0(N,\overline{\omega})$, where $T_0(N,\omega)\equiv\hbar\omega/k_B[N/\zeta(3)]^{1/3}$ is the theoretical transition temperature for an ideal, trapped Bose gas and $\overline{\omega}=(\omega_\rho^2\omega_z)^{1/3}$ [8]. The ordinate is the excitation frequency expressed in units of ω_ρ. Our results were obtained using the experimental value of T, and a value of μ that yielded the experimentally determined value of N. Thus, as for our previous treatment of zero-temperature excitation spectra [7], *this calculation contains no adjustable parameters*. The agreement between theory and experiment is very good (on the order of 5%) for low and intermediate temperatures ($T'\leqslant 0.65$). It should be noted that, as depicted in Fig. 2, the high end of this temperature range corresponds to a non-condensate fraction of about 50%. However, as the temperature increases, the HFB-

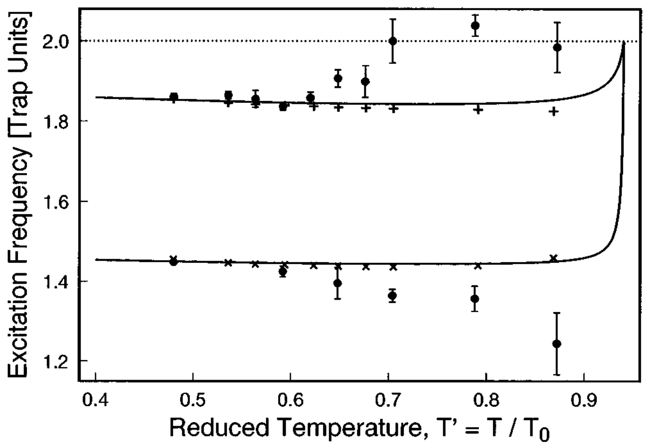

FIG. 1. The experimental, temperature-dependent excitation spectrum in the JILA TOP trap (filled circles) versus the HFB-Popov predictions for the $m=0$ mode (top, labeled by $+$) and the $m=2$ mode (bottom, labeled by $\times$). The solid curves are excitation frequencies for a *zero-temperature* condensate having the same number of condensate atoms as the experimental condensate in the finite-T cloud.

Popov excitation frequencies diverge from the experimental data. This feature of the comparison holds true for both $m=0$ and $m=2$ modes.

The behavior of the calculated excitation frequencies can be understood in a simple way. The HFB-Popov equations determine the equation of state for the state variables $\{N,N_0,T\}$, so that, given the values of N and T, a unique N_0 is determined. For fixed N, this relationship generates the condensate fraction N_0/N as a function of T, which is shown in Fig. 2 for the JILA TOP trap with $N=2000$. One can easily predict the temperature-dependent mode frequencies for the $N=2000$ system by finding the number of condensate atoms, N_0, from Fig. 2, and then determining the *zero-temperature* excitation frequency of a condensate with N_0 atoms, which is a much simpler calculation.

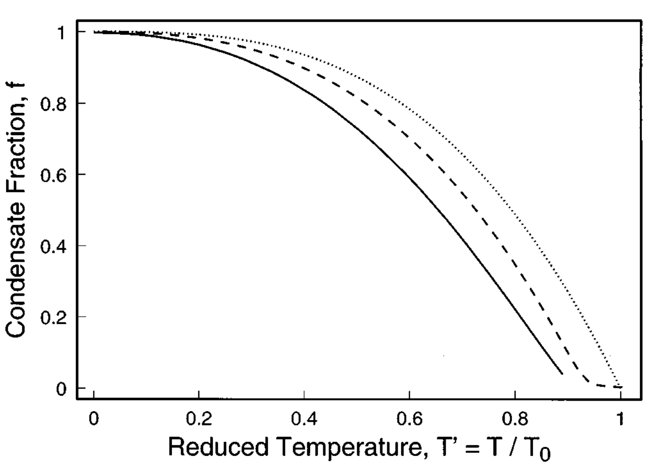

FIG. 2. A plot of the condensate fraction as a function of T' (solid curve) for the JILA TOP trap in which N is fixed at 2000 atoms. The same quantity is shown for the ideal gas in the thermodynamic limit (dotted curve) and for 2000 atoms (dashed curve) for comparison.

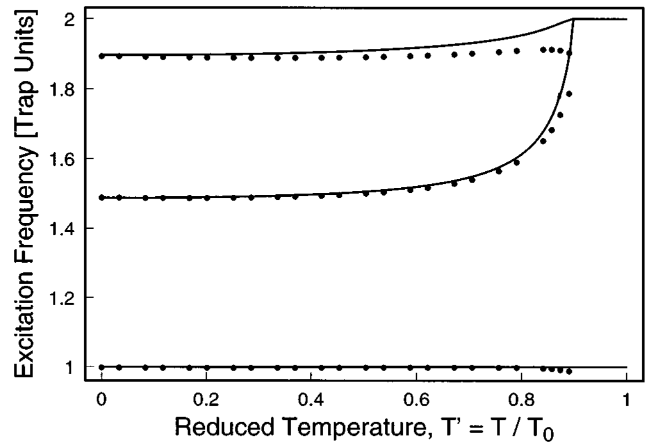

FIG. 3. HFB-Popov excitation frequencies (filled circles) for the $m=0$ (top), $m=2$ (middle), and the $m=1$ modes (bottom) for a cold-atom cloud having $N=2000$ atoms. Overlaid (solid lines) are the frequencies for a zero-temperature system with the same number N_0 of condensate atoms as in the finite-temperature system.

Figure 3 shows a comparison of the three lowest frequencies numerically determined from the HFB-Popov equations, and by the equivalent $T=0$ method just described. The agreement of these two approaches is very good over nearly the entire temperature range. The two solid curves in Fig. 1 are the frequencies determined by the same procedure, except that the number of condensate atoms was taken from experiment. In short, the principal effect of finite temperature on the HFB-Popov excitation spectra is largely an effect of *condensate depletion*: the dynamics of the finite-temperature condensate are essentially the same as those of a zero-temperature condensate with the same value of N_0. This is consistent with earlier calculations [16,17] of the speed of sound in a homogeneous Bose-condensed gas, which found that its temperature dependence was effectively a condensate-density dependence. We discuss this result in a broader context in a separate paper [18], in which we show that HFB-Popov results can be reproduced quantititatively by a much simpler ''two-gas'' model: the condensate gas, which is described by the zero-temperature GP equation; and the thermal cloud, which is described as an ideal Bose gas in an effective potential created by the condensate. This effective potential repels the thermal gas from the condensate gas, which results in the essential independence of temperature of all condensate properties except N_0. Application of simple quantum-statistical mechanics to this model can generate the full phase diagram of Fig. 2 directly.

As Fig. 1 clearly shows, the HFB-Popov solutions reproduce the experimental results quite well when $T \leqslant 0.65 T_0$, but fail at higher temperatures. The HFB-Popov formalism is biased toward a description of the condensate, as it represents the condensate excitations as taking place in a static thermal cloud. Indeed, the HFB-Popov equations can be derived from a generalized time-dependent Gross-Pitaevskii equation that contains a time-independent thermal-density term. This results in at least one minor failure of the approach, which is weakly visible in Fig. 3 as a deviation of the $m=1$ mode frequency from unity near T_0, in violation of the generalized Kohn theorem for parabolic confinement [13,19]. This mode should correspond to a rigid oscillation of the complete N-atom system, and the deviation of its frequency from unity results from the HFB-Popov approximation holding the thermal component fixed and allowing only the condensate to oscillate. In experiments of the type discussed here, however, the thermal component and condensate must both be driven by the modulation of their common confining potential. For other, nonrigid oscillations we may thus also expect thermal and condensate modes to be coupled in general. Thus, HFB-Popov frequencies will only correspond to the experimental values if the condensate response to mechanical disturbance does not induce modulations of the thermal density, so that there is no back action of the thermal cloud on the condensate motion. A more general theory that accounts for such condensate-cloud interactions has recently been outlined [20], but remains to be implemented. The self-consistent inclusion of pair terms, which are neglected in the Popov approximation, may also be important for capturing multiple-collision effects in the theory of trapped BECs [21]. The effect of such terms can be very marked close to the transition temperature [22].

In conclusion, we have delineated the region of validity of the Popov version of finite-temperature HFB theory by comparing it directly with the results of recent experiments. Good agreement is obtained for condensate fractions from unity down to about 0.5, so the HFB-Popov is apparently correctly describing finite-temperature phenomena in a nontrivial regime. This comparison confirms the critical role of evaporatively cooled gases in establishing proper finite-temperature field theories of Bose-Einstein condensation, and shows that there is still work needed to establish satisfactory agreement between theory and experiment for cases of small condensate fraction.

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